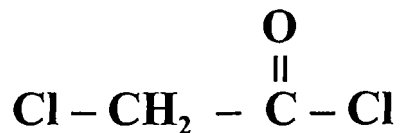


AEGLs for CHLOROACETYL CHLORIDE (CAC)

ORNL Staff Scientist: Sylvia Milanez

Chemical Manager: Steven Barbee

Chemical Reviewers: Nancy Kim and Robert Benson

-
- ▶ Chloroacetyl chloride (CAC) is a liquid with a pungent odor. It decomposes exothermally in water to produce chloroacetic acid and HCl.
 - ▶ CAC major uses are as an intermediate in the synthesis of tear gas, chloracetamide herbicides, and pharmaceuticals. In 1992 >45,000 metric tons were used industrially.
 - ▶ CAC is corrosive to tissues and irritates the eyes, skin, and respiratory system. Secondary sources report the vapor can cause dyspnea, cough, cyanosis, laryngospasm, pulmonary edema, bronchospasm and bronchopneumonia.

CHLOROACETYL CHLORIDE (CAC)

HUMAN TOXICITY DATA

- ▶ **No acute lethality studies**

- ▶ **Odor Awareness:**
 - ▶ **0.011 ppm** was undetectable (1 hygienist; Dow, 1988b),
 - ▶ **0.023 ppm** was barely detectable (“”)
 - ▶ **0.140 ppm** was “strong” (“”)
 - ▶ **0.05 ppm**, collected over ≥ 7 hrs, was “readily apparent and objectionable” (Monsanto 1987)

- ▶ **Irritation:**
 - ▶ **0.91 ppm** was painful to the eyes and caused lacrimation (Dow 1988b)
 - ▶ **0.43 ppm** was threshold of irritation (Lim_{ir}) for humans “using subjective indicators” (Germanova et al. 1988). Exposure time not reported, possibly 1 min, per Izmerov et al. (1982) definition.

Chloracetyl Chloride Inhalation Single-Exposure Animal Studies					
Species	Exp. time (Ref.)	Conc. ¹ (ppm)	Mortality		Effects, Comments
			M	F	
Rat	1 hr (Dow '86)	32 [AEGL-2]	0/6	0/6	► Eye squinting, lacrimation during exposure; urine stains, initial weight loss
		208	0/6	0/6	► As at 32 ppm but worse; also shallow breathing; lethargy, periocular red stains
		522	0/6	0/6	► As at 208 ppm but worse; labored breathing, gasping, salivation, red stains near muzzle
		747	5/6	1/6	► LC ₅₀ = 660 ² or 645 ³ ppm for M; death on d. 2, 7, 8, 13 (F); toxicity as for 522 ppm but worse, lung edema or lungs don't collapse at necropsy, enlarged adrenals
Rat	2 hrs(Herzog'59)	108-6494 (N)	100% at ≥3462		► 80 animals tested, obs. 5 d.; sex, strain, # rats/group, and specific results not given.
Rat	4 hrs (Carp. '49)	1000 (N)	2/6, 3/6, or 4/6		► Animal sex and further methods and results details were not provided.
Rat	7 hrs 5-10 min	~2.5 ~4	0/? 0/?		► No visible effects; # and sex rats not stated ► Respiratory distress; "" (Dow'70a)
Mouse, white	2 hrs (Herzog 1959)	108 -6494 (N)	0/10 to 10/10		► LC ₅₀ = 1066 ppm; mice obs. only 5 days. All had upper respiratory irritation (rubbed mouth, half-open and watery eyes, dyspnea). Most lesions in trachea & lungs (edema, hemorrhage, necrosis). Tox. not stated for specific concs.
Guinea pig	2 hrs (Herz.'59)	108-6494 (N)	100% at ≥3462		► 50 animals; obs. 5 d. Sex, strain, #animals/group, and specific results not given.

¹Exposure concentrations are **analytical** unless stated otherwise (N=nominal).

TABLE 3. Chloracetyl Chloride Dow 1982 Multiple-Exposure Animal Study

Species	Exposure time	Conc. (ppm)	Mortality		Effects, Comments
			M	F	
Rat	4 wks, 6 hr/d, 5d/wk	0.5 ² [AEGL-1]	0/10	0/10	▶ Conjunctival redness after initial exp., olfactory epithelium inflammation
		1.0	0/10	0/10	▶ As at 0.5 ppm but worse, nasal exudate, poor weight gain, lung lesions
		2.5	8/10	9/10	▶ As at 1 ppm but worse, lethargy, BW loss, lesions in nasal turbinates, trachea, and/or lungs (inflammation, hypertrophy, -plasia, metaplasia, necrosis, atrophy, pneumonitis or bronchitis). No death 1 st wk.
		5.0	10/10	9/10	▶ As at 1 ppm but worse. No death 1 st wk.
Mouse	4 wks, 6 hr/d, 5d/wk	0.5 ²	0/10	0/10	▶ Sneezing, conjunctivitis, resp. mucosa inflammation w. eosinophilic inclusions in nasal turbinates, trachea, and bronchi
		1.0	0/10	0/10	▶ As at 0.5 ppm but worse, poor weight gain
		2.5	0/10	2/10	▶ As at 1 ppm but worse, BW and fat loss, mucosal hypertrophy and hyperplasia. No death 1 st wk.
		5.0	1/10	2/10	▶ As at 2.5 ppm but worse, rales, lethargy, nasal exudate, alveolar macrophages w. red cytoplasmic masses. No death 1 st wk.
Hamster	4 wks, 6 hr/d, 5d/wk	0.5 ²	0/10	0/10	▶ Sneezing and closed eyes
		1.0	0/10	0/10	▶ As at 0.5 ppm but worse
		2.5	0/10	0/10	▶ As at 1 ppm but worse, poor weight gain
		5.0	0/10	0/10	▶ As at 2.5 ppm but worse, weight/fat loss

CHLOROACETYL CHLORIDE (CAC)

AEGL-1

Key Study: Dow 1982. Endpoint: Mild eye irritation (conjunctival redness) in rats after a single 6-hour exposure to ~1 ppm (0.84 ± 0.51 ppm).

Scaling: None; using the same value across time was considered appropriate since mild irritant effects do not vary greatly over time

Total Uncertainty Factor: 10

Interspecies: 3: Eye conjunctivitis due to local contact irritation is not expected to vary greatly among animals

Intraspecies: 3: Eye conjunctivitis due to local contact irritation is not expected to vary greatly among humans

AEGL-1 Values for Chloroacetyl Chloride (CAC)				
10-min	30-min	1-hr	4-hr	8-hr
0.08 ppm	0.08 ppm	0.08 ppm	0.08 ppm	0.08 ppm

► **AEGL-1 is supported by the limited human data:**

- It is **>0.05 ppm**, which had an “objectionable” odor throughout a ≥ 7 hr work shift, but no any adverse health effects were reported.
- It is ~10-fold below **0.9 ppm**, which was “painful” and caused lacrimation
- It is comparable to **0.140 ppm**, which had “strong” odor but was not irritating to the eyes upon exposure for a few (??) minutes (noting that an intraspecies UF=3 would lower 0.14 ppm to **0.05 ppm**).

CHLOROACETYL CHLORIDE (CAC)

AEGL-2

Key Study: Dow 1986. Toxicity endpoint: eye lacrimation and eye squinting, which would impede the ability to escape. The point of departure was 32 ppm because the next higher conc. tested (208 ppm) was near the estimated lethality threshold of 215 ppm for rats.

Time scaling: $C^n \times t = k$ (ten Berge et al. 1986); no data to derive n; scaled using n=3 for <1 hr and n=1 for >1 hr, exc. for 8 hrs adopted 4-hr value because calculated 8-hr value (0.13 ppm) is near the AEGL-1 (0.08 ppm).

Total Uncertainty Factor: 30

Interspecies: 10: Data suggests humans are more susceptible to lacrimation from CAC exposure than animals**.

Intraspecies: 3: Lacrimation due to severe local contact irritation is not expected to vary greatly among humans.

[**0.9 ppm caused lacrimation and eye pain in human (??time), but rats, mice and hamsters exposed to 5 ppm for 6 hrs/day had conjunctivitis w/o lacrimation]

AEGL-2 Values for Chloroacetyl Chloride				
10-min	30-min	1-hr	4-hr	8-hr
1.9 ppm	1.3 ppm	1.1 ppm	0.27 ppm	0.27 ppm

- ▶ AEGL-2 values are supported by the limited human data (see AEGL-1)

CHLOROACETYL CHLORIDE (CAC)

AEGL-3

Key Study: Dow 1986. Toxicity endpoint: the lethality threshold, estimated as 215 ppm (1/3 of the LC_{50} for male rats)

Time scaling: $C^n \times t = k$ (ten Berge et al. 1986); no data to derive n ; scaled using $n=3$ for <1 hr and $n=1$ for >1 hr.

Total Uncertainty Factor: 10

Interspecies: 3: Lethality from respiratory lesions and having a steep dose-response occurred in several rat and mouse studies, at CAC concs. within a factor of 2-3

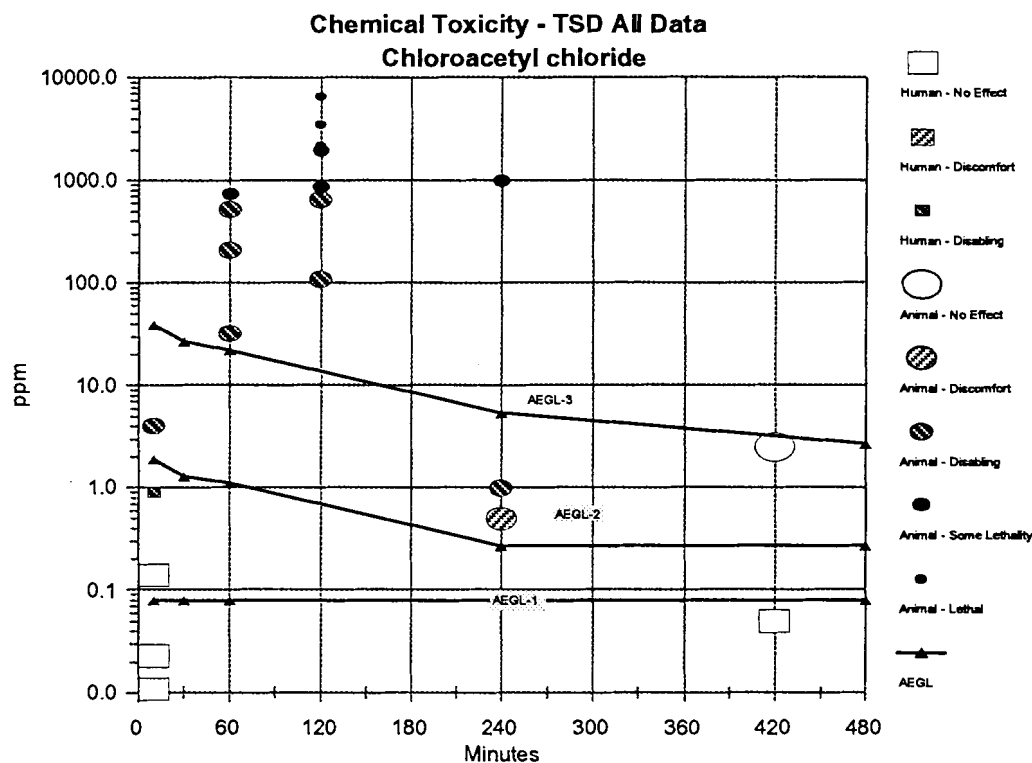
Intraspecies: 3: Threshold for lethality from direct destruction of respiratory tissue is not expected to vary greatly among humans, based on steep dose-response seen in the animal studies.

AEGL-3 Values for Chloroacetyl Chloride				
10-minute	30-minute	1-hour	4-hour	8-hour
39 ppm	27 ppm	21 ppm	5.4 ppm	2.7 ppm

Summary of AEGL Values for Chloroacetyl Chloride (ppm)						
Classification	10-min	30-min	1-hr	4-hr	8-hr	Endpoint (Reference)
AEGL-1^a (Non-disabling)	0.08	0.08	0.08	0.08	0.08	Conjunctival redness in rats (Dow 1982)
AEGL-2 (Disabling)	1.9	1.3	1.1	0.27	0.27	Lacrimation and eye squinting in rats (Dow 1986)
AEGL-3 (Lethal)	39	27	21	5.4	2.7	Threshold for lethality in male rats (Dow 1986)

^a Odor of 0.023 ppm was reported to be barely detectable by an industrial hygienist (Dow 1988b).

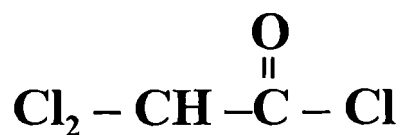
Category Plot for Chloroacetyl Chloride



Notes:

1. For Dow 1982 multiple-exposure study, one 6-hour exposure to 0.5 ppm was entered as Category 1 (discomfort) for rats, mice, and hamsters. A single 6-hour exposure to 1 ppm was entered as Category 1 only for rats.
2. For Dow 1988b human study, exposure time was not defined, and was estimated to be 10 minutes for the Category plot.
3. Analytical concentrations are presented if available. No adjustments were made for discrepancies between nominal and analytical concentrations (latter were 45-82% lower than nominal in studies where both were stated).

AEGLs for DICHLOROACETYL CHLORIDE (DCAC)



ORNL Staff Scientist: Sylvia Milanez

Chemical Manager: Steven Barbee

Chemical Reviewers: Nancy Kim and Robert Benson

- ☐ Dichloroacetyl chloride (DCAC) is liquid with an acrid, penetrating odor. It decomposes in water to form HCl and dichloroacetic acid.
- ☐ DCAC is irritating to the eyes and mucous membranes. Acute exposure may cause dyspnea, chest pain, upper airway and pulmonary edema, bronchospasm, pneumonitis, airway hyper-reactivity, and chronic lung function abnormalities.
- ☐ DCAC production in the U.S. exceeds 1 million pounds annually; it is mainly used as a reactive intermediate.
- ☐ No standards or guidelines are currently available for DCAC air exposure.

DICHLOROACETYL CHLORIDE (DCAC)

HUMAN TOXICITY DATA

☐ **No acute lethality studies**

☐ **Non-lethal toxicity:** Dahlberg and Myrin (1971) described 10 welding shop scenarios; only two reported workers' responses (#3 and #6). DCAC (and phosgene) was formed from welding arc in air cont. trichloroethylene (TCE). Air samples collected 3 min, ~30 cm from the arc. Conclusions:

- ☐ **0.1 ppm:** DCAC odor is recognized
- ☐ **0.5-1 ppm:** exposures above this conc. not advisable; workers may tolerate for a time without complaining except of "bad smell,"
- ☐ **10 ppm:** caused immediate coughing and eye irritation and is not endurable for long", and
- ☐ **13 ppm:** "could certainly not be endured for 1 hr" [**Scenario 3**]

Shop	DCA C	Phosg.	TCE	Scenario description
	(ppm)			
#3 [Near welding site; near vent]	13 0.5		256 248	Welding was ~ 10 m from spill of ~10 L TCE, which was swept into a drain. Simulated accident; ~1 hr exposure. Worker noticed unpleasant smell, left to vomit, came back, and lost consciousness. He was hospitalized and quickly regained consciousness. Afterwards, he had muscular pains and was "sick listed" for a "long time."
#6 [Before & after fan adjustment]	10.4 1.6	0.3 0.06	65 27	TCE source was 15-20 m from unventilated welding bench. All nearby noticed "very disagreeable smell" and the welder had several coughing attacks.

☐ Phosgene was produced at ~5x lower amount than DCAC. The welders' symptoms are believed due to DCAC because: (1) TCE has a sweet odor, detectable at ≥ 50 ppm, and (2) phosgene has a mild odor perceptible at 0.4 ppm, and causes throat and ocular irritation at ≥ 3.1 - 4.8 ppm.

DICHLOROACETYL CHLORIDE (DCAC)

ANIMAL TOXICITY DATA

Acute Lethality:

- ☐ Range-finding test: 2/6 rats (M?) died after inhaling 2000 ppm DCAC for 4 hrs (nominal conc.; Smyth et al. 1951). Inferred that 0/6 died at 1000 ppm based on methodology [tested log series of concs. with a factor of two, and reported results only for fractional mortality]. No other effects reported.
- ☐ Smyth et al. (1951) exposed 6 rats to ~saturated DCAC vapor (30,000 ppm). Longest period survived by all rats was 8 minutes.

Nonlethal Toxicity:

- ☐ Carcinogenicity study: M rats (50/dose) given 30 exposures of 0.5, 1.0, or 2.0 ppm DCAC for 6 hours/day, 5 days/week had no mortality during treatment; 2/50 exposed to 2.0 ppm developed nasal carcinomas (none in control group; Sellakumar et al. 1987). Cageside observations, gross pathology, body weights not reported.

The anterior respiratory epithelium was the most severely affected: saw necrosis, ulceration, acute inflammation, and in some cases squamous metaplasia and dysplasia.

DICHLOROACETYL CHLORIDE (DCAC)

AEGL-1

- ☐ **Not recommended due to insufficient data.** No human or animal studies were conducted in which endpoints consistent with the definition of AEGL-1 were reported.
- ☐ Exposure to 0.1 ppm DCAC, which was stated to have a recognizable odor in the welding shop study (Dahlberg and Myrin 1971), was not associated with a specific exposure duration or adverse health effects.

DICHLOROACETYL CHLORIDE (DCAC)

AEGL-2

Key Study: Welder shop scenario: workers exposed to ~1.6-10.4 ppm DCAC noticed a “very disagreeable smell” and the welder had several coughing attacks (Dahlberg and Myrin 1971). Exposure duration not reported; but est. as 10 min (each welding operation took only few min.)

Toxicity endpoints: Coughing and notable discomfort at 1.6 ppm

Time scaling: $C^n \times t = k$ (ten Berge et al. 1986); no data to derive n ; used $n=1$ to scale to 30 min. Same value adopted for 30 min to 8 hrs because scaling to ≥ 1 hr yielded concs. below those recognized by workers (i.e. 0.1 ppm).

Total Uncertainty Factor: 3

Interspecies: Not applicable

Intraspecies: 3: The key toxic endpoint (coughing; notable discomfort) is not likely to be significantly worse in the general population than in repeatedly exposed workers.

AEGL-2 Values for DCAC				
10-minute	30-minute	1-hour	4-hour	8-hour
0.53 ppm	0.18 ppm	0.18 ppm	0.18 ppm	0.18 ppm

- ☐ Key study also states that exposures to >0.5-1 ppm are “not advisable” but may be tolerated “for a time” w/o complaining except of “bad smell”.

DICHLOROACETYL CHLORIDE (DCAC)

AEGL-3

Key Study: Smyth et al. (1951) range-finding test: 2/6 rats exposed to 2000 ppm for 4 hours died, whereas 0/6 rats died at 1000 ppm (nominal concentration; estimate 500 ppm as analytical concentration), which is an estimated lethality threshold. No results other than death were reported.

Toxicity endpoint: The estimated lethality threshold (500 ppm)

Time scaling: $C^n \times t = k$ (ten Berge et al. 1986); no data to derive n ; used $n=3$ and $n=1$ to extrapolate to < 4 hours and > 4 hours, respectively, except 30-min values were adopted as 10-min values.

Total Uncertainty Factor: 100

Interspecies: 10: Only one species tested; cause of death in key study not defined.

Intraspecies: 10: Because cause of death in the key study was unknown, variability among humans cannot be reliably estimated.

Modifying factor: 2: The analytical conc. was not provided, and may be half the nominal conc. based on study with related compd. CAC

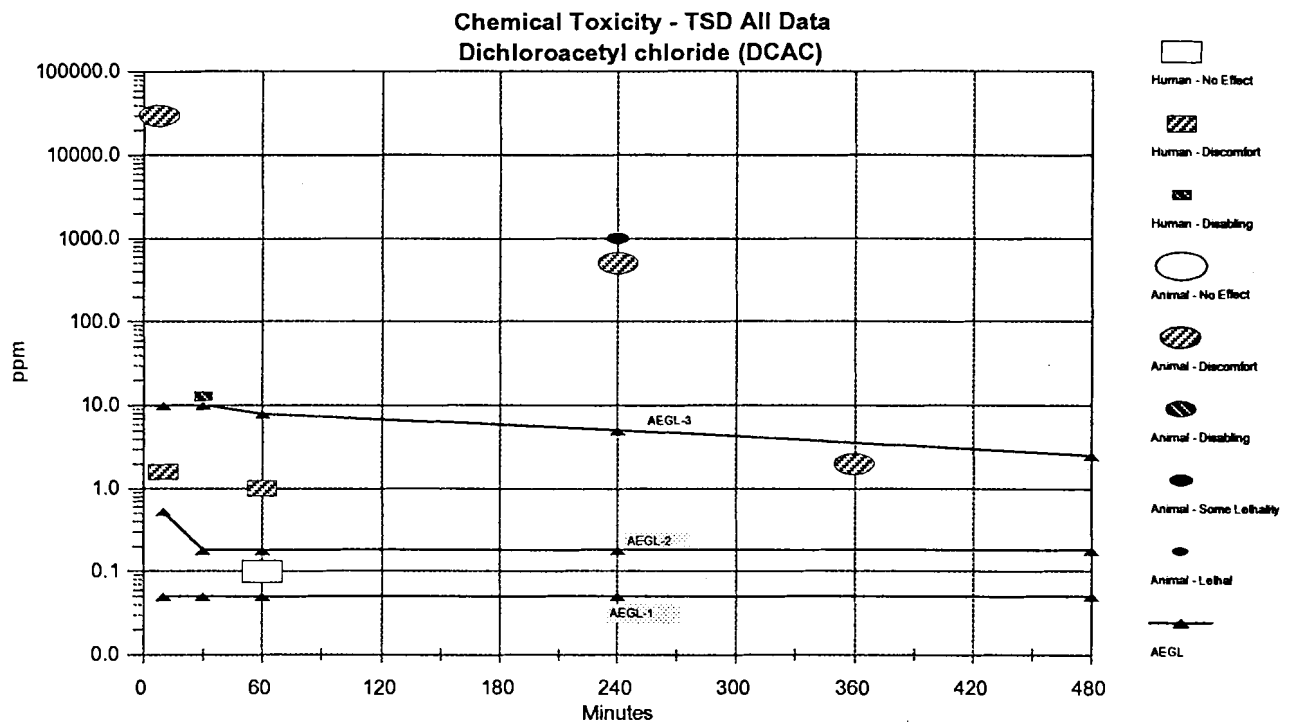
AEGL-3 Values for DCAC				
10-minute	30-minute	1-hour	4-hour	8-hour
10 ppm	10 ppm	7.9 ppm	5.0 ppm	2.5 ppm

- ☐ AEGL-3 values are consistent with human welder scenario, in which a worker exposed to ~13 ppm for ~1 hr lost consciousness, recovered in hospital, but had muscular pains and was unable to work for a long time.

Summary of AEGL Values for DCAC						
Classifi- cation	10-min	30-min	1-hr	4-hr	8-hr	Endpoint (Reference)
AEGL-1 ^a (Non-disab)	Not recommended due to insufficient data.					
AEGL-2 (Disabling)	0.53	0.18	0.18	0.18	0.18	Coughing and notable discomfort in workers (Dahlberg and Myrin '71)
AEGL-3 (Lethal)	10	10	7.9	5.0	2.5	Threshold for lethality in rats (Smyth et al. 1951)

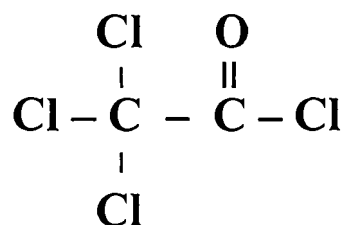
^a Odor is recognized at 0.1 ppm.

Category Plot for Dichloroacetyl Chloride



Note: AEGL-1 values were not recommended due to insufficient data; but assumed a value of 0.05 to be able to generate this plot.

AEGLs for TRICHLOROACETYL CHLORIDE (TCAC)



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Chemical Manager: Robert Benson

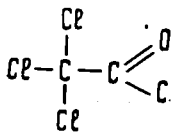
Chemical Reviewers: Nancy Kim and Steven Barbee

-
- TCAC is a corrosive liquid with a pungent odor. Decomposes in water to produce trichloroacetic acid and hydrochloric acid (HCl)
 - Used as intermediate in organic synthesis; no information on annual production volume
 - No odor threshold data, air standards, or guidelines available
 - Causes irritation of the eyes, skin, and respiratory system, possibly leading to spasm, inflammation, edema of the larynx or bronchi, chemical pneumonitis, and pulmonary edema.

TRICHLOROACETYL CHLORIDE (TCAC)

**AEGL-1, AEGL-2, and AEGL-3 values not recommended
due to insufficient data.**

The only available data was a secondary report (Izmerov et al. 1982) that provided no details of the study methods or results, and which was not considered appropriate for AEGL derivation.

<p>Trichloroacetyl chloride+</p>  <p>MAC_{wz} 0.1 (v), Class I 248, 461</p>	<p>Intragastric: LD₅₀ rat 600 Inhalation: LC₅₀ rat 475 (318—698) 4 h, LC₅₀ mouse 445 (296—667); Lim_{ac} rat 10 4 h (1, 11, 15), Lim_{ac} rat 1—3 4 h (7, 9); Lim_{ir} man 0.6 Has irritant properties Detection: colorimetry; detection limit 0.1 µg in analytical volume</p>
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TCAC : Data from *Izmerov et al. 1982*

- Lim_{ir} (irritation threshold) for humans was 0.08 ppm. This was not used to derive AEGL-1 values because the original study and methods details were unavailable, and the exposure duration (1 minute) was insufficient.

[Lim_{ir} = “the threshold of irritant action on the mucous membranes of the upper airways and eyes. Values for man are based on subjective sensations for exposures lasting 1 min unless stated otherwise.”]

- LC_{50} of 64 and 60 ppm were reported for 4-hr exposure for rats and mice. These stand-alone values were not used to derive AEGL-3 values because the original study (with the respective methods and results details) was unavailable.
- For the same reason, the stand-alone LC_{50} values were not used to derive AEGL-2 values by applying an adjustment factor.

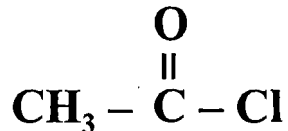
TCAC : Data from Izmerov et al. 1982

- Lim_{ac} (“threshold of acute effect”) for rats for 4-hr exposure was 1.34 ppm [based on changes in the summation threshold index, rectal temperature, and motor activity] and 0.13-0.40 ppm [based on changes in respiration rate and lung staining].
- While some of these effects may be within the scope of AEGL-2, the lack of methods and results details precluded use of the data for AEGL-2 derivation.

[Lim_{ac} = “lowest concentration (dose) that causes such a change in a particular biochemical index in a whole organism which is beyond the latter’s capacity for physiological adaptation.”]

**THEREFORE: AEGL-1, AEGL-2, and AEGL-3 values
were NOT recommended due to
insufficient data.**

AEGLs for ACETYL CHLORIDE (AC)



ORNL Staff Scientist: Sylvia Milanez

Chemical Manager: Steven Barbee

Chemical Reviewers: Nancy Kim and Robert Benson

- ✓ AC is a colorless, flammable, fuming liquid with a pungent odor
- ✓ Decomposes in water to form hydrogen chloride (HCl) and acetic acid
- ✓ AC is a severe eye and respiratory tract irritant. Can cause spasm, inflammation, and edema of larynx and bronchi, chemical pneumonia, pulmonary edema.
- ✓ Has many uses as acetylating agent, e.g. in pharmaceutical manufacture. No data for U.S. production volume; U.S. market is ~ 500 tons annually.

ACETYL CHLORIDE (AC)

**AEGL-1, AEGL-2, and AEGL-3 values not recommended
due to insufficient data.**

HUMAN TOXICITY DATA

- ✓ No quantitative Acute Lethality data were located.
- ✓ No odor threshold data
- ✓ No air standards or guidelines are currently available.
- ✓ Two anecdotal (i.e. no experimental data) reports:
 - ✓ Inhalation of 2.3 ppm AC for one min was intolerable (NAMCC 1961)
 - ✓ 0.5 ppm AC causes lacrimation and a burning sensation in eyes, nose, and throat (Wagner 2002; no additional details provided.

ANIMAL TOXICITY DATA

- ✓ No animal studies with AC were located.

Summary of AEGL Values for Chloroacetyl Chloride (ppm)						
Classification	10-min	30-min	1-hr	4-hr	8-hr	Endpoint (Reference)
AEGL-1 ^a (Non-disabling)	0.08	0.08	0.08	0.08	0.08	Conjunctival redness in rats (Dow 82)
AEGL-2 (Disabling)	1.9	1.3	1.1	0.27	0.27	Lacrimation and eye squinting in rats (Dow 86)
AEGL-3 (Lethal)	39	27	21	5.4	2.7	Threshold for lethality in male rats (Dow 86)

^aOdor of 0.023 ppm was barely detectable; 0.05 ppm was “objectionable”; 0.14 ppm was “strong” to an industrial hygienist.

Summary of AEGL Values for DCAC						
Classifi-cation	10-min	30-min	1-hr	4-hr	8-hr	Endpoint (Reference)
AEGL-1 ^a (Non-disab)	Not recommended due to insufficient data.					
AEGL-2 (Disabling)	0.53	0.18	0.18	0.18	0.18	Coughing and notable discomfort in workers (Dahlberg and Myrin '71)
AEGL-3 (Lethal)	10	10	7.9	5.0	2.5	Threshold for lethality in rats (Smyth et al. 1951)

^a Odor is recognized at 0.1 ppm.

TABLE X-1. Comparison of physical, chemical, and toxicological values for the acetyl chlorides and their hydrolysis products					
Parameter	Acetyl chloride (AC)	Chloroacetyl chloride (CAC)	Dichloroacetyl chloride (DCAC)	Trichloroacetyl chloride (TCAC)	HCl
Molecular weight (CAS#)	78.50 (75-36-5)	112.94 (79-04-9)	147.39 (79-36-7)	181.83 (76-02-8)	36.46 (7647-01-0)
Solubility in water	decomposes	decomp. $t_{1/2}$ <30min	decomposes, $t_{1/2}$ 0.004 min	decomposes; 9.49 g/L @ 25°C	soluble
Vapor pressure	287 mm Hg @25°C	20 mm Hg @ 21°C	23mm Hg @ 25°C	21.3mm Hg@ 25°C	4.0 @ 17.8°C
Vapor density (air =1)	2.7	3.9	5.1	Not found	1.639
Liquid density (H ₂ O=1)	1.11	1.42 @ 20°C	1.5315 @ 16°/4°C	1.654 @ 0°/4°C	1.19 (38% soln.)
Odor and Irritation data (ppm)	no odor data; h: 0.5 lacrimation, 2.3 1 min intolerable	pungent; h: 0.023 barely detect; 0.9 lacrimation, pain	acidic; recog 0.1 ppm	no odor data; h: 0.08 is 1 min irrit. threshold	odor thr 1-5; ≥5 irr.; 50-100 max tol. for prolonged period
Lethality data – LC ₅₀	not found	660 rat 1 hr	>2000 ppm 4 hr rat	rat 64ppm 4h; mus 60 ppm ??h	Rat 1 hr 3124; mus 1 hr 1108
Lethality data – LD ₅₀	rat 910 mg/kg		2460 mg/kg	600 mg/kg rat	900 mg/kg rabbit
Corresponding ACID	acetic	chloroacetic	dichloroacetic	trichloroacetic	
Molecular weight (CAS#)	60.06 (64-19-7)	94.5 (79-11-8)	128.94 (79-43-6)	163.39 (76-03-9)	
pKa (pH 0.1 M solution)	4.756	2.87 (pH 1.93)	1.26	0.51 (pH 1.2)	None (<0; completely dissociates)
Water solubility	infinite; miscible	6.14 kg/L	1 kg/L	1.3 kg/L	
Vapor density (air =1)	2.07	3.26	4.45	Not available	
Liquid density (H ₂ O=1)	1.049	1.404	1.5724	1.6298	
Vapor pressure (mmHg)	11.4@20°C	0.06 @25°C	0.18 @25°C	4.54E-9 @25°C,	
Odor and Irritation data (ppm)	pungent; TCLO hum 816	~vinegar, 50% recog 0.045; Irrit h: 1.48; rat 6.16, NOEL 0.31, 0.13	H recog 0.04	H recog 0.24-0.37	
Lethality data – LC ₅₀ (ppm)	LCLO rat 16,000 4 h mus LC50 5620 1h	rat 47 ppm 4 hr	not found	rat, rabbit, cat, g. pig 4 hrs >4800 ppm	
Lethality data – LD ₅₀ (mg/kg)	3310 mg/kg rat	rat 108, 76, 580; pig 80 mg/k; 165 mg/kg	2820 mg/kg rat	dog 1600-2000, rat 3310-6900, mus 4970	